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Institute of Mathematical Sciences
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Upper Bounds on Scattering Lengths When Composite Bound States Exist

L. ROSENBERG, L. SPRUCH and T. F. O'MALLEY

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Abstract

In the case of the zero energy scattering of one compound system by another, where one real scattering length completely characterizes the problem, (e.g., the reaction A+B → C+D, in addition to A+B → A+B, cannot take place) it has previously been shown that the Kohn-Hulthén variational principle provides an upper bound on the scattering length if no composite bound states exist. The extension of this result to the case where one or more composite bound states do exist is presented here. The inclusion of tensor forces, exchange forces, and Coulomb forces is allowed. Several methods are given for obtaining a rigorous upper bound on the scattering length, which involve the addition of certain positive terms to the Kohn-Hulthén variational expression. The approximate information about the composite bound states which is required to construct these additional terms can be found by standard methods. As a consequence of one of the results obtained, it is shown that under certain circumstances some ordinary variational calculations give a bound. Thus, an analysis of a previous calculation in the light of the present results leads, without further calculations, to a rigorous upper bound on the singlet electron-hydrogen scattering length.

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I. INTRODUCTION

The value of variational methods in scattering problems is greatly increased when these methods are based on a minimum (or maximum) principle. This is especially true for the difficult case of scattering by a compound system, where calculations in which different trial functions are used can lead to quite different results. Such a minimum principle, for zero energy scattering, has already been obtained for the case in which the scattered particle cannot be bound to the scattering system[1]. The present paper is concerned with the extension of this result to the case in which one or more composite bound states exist. For clarity of presentation the detailed discussion is confined to the problem of the scattering of a spinless, neutral particle, of zero orbital angular momentum, from a short range center of force. The generalization to the case where the scattering is by a compound system, and where long range Coulomb forces exist, is identical with the corresponding generalization in the problem in which no composite bound states exist[2], and the details will be omitted. Further, the inclusion of tensor forces is allowed. The formulation, given in II, for the scattering of a particle by a compound system can be extended, in a straightforward way, to treat the scattering of one compound system by another. It will in fact be understood in the following that unless otherwise stated (in particular, the result of Section IV is excepted) each of the results obtained has, under the condition discussed in II, direct applicability to this wider class of problems (the essential requirement is that the scattering be completely characterized by one real scattering length). The problems which may be treated include zero energy scattering of a neutron or a proton (or in fact of nuclei) by nuclei, assuming realistic nuclear potentials. Similarly, the scattering of electrons (or atoms) by atoms may be treated.

As discussed in II, the scattering cannot be characterized by a real

scattering length if the radiative capture process is possible. We shall, in the following, make the approximation of ignoring the interaction of the particle with the radiation field. The bound on the scattering length is then rigorous only to the extent that this generally excellent approximation is in fact valid.[3]

In Section II a number of results are obtained which provide upper bounds on the scattering length for the case where only one bound state exists. In Section III it is shown that there are well defined circumstances for which some ordinary variational calculations provide a bound. An alternate method for obtaining bounds, based on the Kato formalism, is considered in Section IV. The extension to the case of many bound states is treated in Section V. Since in this case the exact scattering function has a number of nodes (even for the scattering of a particle by a center of force), making the construction of an accurate trial function more difficult, it would seem that a minimum principle for the scattering length is even more valuable here.

II. THE CASE OF ONE BOUND STATE

We begin by considering the problem of the zero energy, zero orbital angular momentum scattering of a spinless neutral particle of mass m by a short range center of force whose strength is such that one, and only one, bound state exists. As shown in I, the scattering length A may, in general, be written

$$A = A_t - \int u_t \mathcal{L} u_t dr + \int w \mathcal{L} w dr \,, \tag{2.1}$$

where u_t is a trial scattering function, w is the difference between u_t and the exact function, u, and $\mathcal{L}$ is defined, in terms of the Hamiltonian, H, as

$$\mathcal{L} = -(2m/\hbar^2)H = \frac{d^2}{dr^2} - (2m/\hbar^2)V(r) \,.$$

(Actually, since we write the one dimensional equations with a factor of 1/r

separated out from the wave function, the differential operator in H is not exactly the kinetic energy operator.) In Eq. (2.1), and in the following, all one dimensional integrals are understood to have the limits zero and infinity. The exact function is determined by the equation

$$\mathcal{L}\, u = 0 \,,$$

with boundary conditions

$$\begin{aligned} &u(0) = 0 \,, \\ &u(r) \to A - r, \quad \text{for } r \to \infty \,. \end{aligned} \tag{2.2}$$

The trial function, u_t, satisfies the same boundary conditions, with A replaced by A_t. It was shown in I that if no bound state exists, and if the normalization given by Eqs. (2.2) (referred to in the following as the "appropriate" normalization) is employed, then

$$\int w \mathcal{L} w \;\leq\; 0 \,, \tag{2.3}$$

so that the Kohn-Hulthén variational expression provides an upper bound on A. The inequality, Eq. (2.3) follows from the fact that under the circumstance considered, the Hamiltonian is positive definite on a space of quadratically integrable functions or, more generally, (see I) for functions which approach some finite, possibly non-vanishing constant at infinity. Thus the inequality will not generally be valid if the asymptotic form for u has what we shall refer to as the " inappropriate" normalization, namely,

$$u \to 1 - r/A, \quad \text{for } r \to \infty. \tag{2.4}$$

We assume in the following that the "appropriate" normalization is employed. (It is of course true that at non-zero energies one cannot generally say which normalization is superior, and that even at zero energy the " inappropriate" normalization provides a variational estimate for if not a bound on the scattering length.)

In the case where one bound state exists, which is our present concern, the inequality, Eq.(2.3), will not be valid unless the error function, $\underline{w}$, is orthogonal to the exact bound state function, denoted by $u_{\varepsilon 1}$, where $(u_{\varepsilon 1} u_{\varepsilon 1}) = 1$. [We have $\mathcal{L} u_{\varepsilon 1} = \varepsilon_1 u_{\varepsilon 1}$, where ε_1 is related to the bound state energy E_1 by $\varepsilon_1 = -(2m/\hbar^2)E_1$.] Since the exact solutions $\underline{u}$ and $u_{\varepsilon 1}$ are orthogonal, the difference function $\underline{w}$ will be orthogonal to $u_{\varepsilon 1}$ provided u_t and $u_{\varepsilon 1}$ are orthogonal. We therefore have the result that the Kohn-Hulthén variational principle gives an upper bound on the scattering length provided a trial function is used which is orthogonal to the exact bound state wave function.

It is easily shown that this statement is equivalent to the expression for the bound given below in Eq. (2.5), where the only requirement on u_t is that it satisfy the correct boundary conditions. However, we will actually obtain Eq. (2.5) in a slightly different way, which is the more natural generalization of the method used for the no bound state case. Although $\underline{w}$ is in fact unknown, we may formally construct a function, namely,

$$[w - (w,u_{\varepsilon 1})u_{\varepsilon 1}],$$

which is orthogonal to $u_{\varepsilon 1}$. It then follows, exactly as in the case for no bound states, that

$$([w-(w,u_{\varepsilon 1})u_{\varepsilon 1}],\mathcal{L}\,[w-(w,u_{\varepsilon 1})u_{\varepsilon 1}]) \leq 0.$$

This inequality may be written

$$(w,\mathcal{L} w) \leq \varepsilon_1 (u_t,u_{\varepsilon 1})^2,$$

where we have made use of the relation $(w,u_{\varepsilon 1}) = (u_t,u_{\varepsilon 1})$. Thus, an upper bound on A may be obtained from

$$A \leq A_t - \int u_t \mathcal{L} u_t \, dr + \varepsilon_1 \left(\int u_t u_{\varepsilon 1} dr\right)^2. \qquad (2.5)$$

The difficulty with Eq. (2.5) is that $u_{\varepsilon l}$ is not known in general. Therefore unless the last term in Eq. (2.5) is small, for a given (presumably) reasonably accurate trial function u_t, and shows very small variation as the accuracy of the trial bound state function, $u_{\varepsilon lt}$, is increased, one cannot claim to have a bound. In fact, preliminary calculations based on Eq. (2.5), for the singlet e^-H problem, gave negative results in the sense that the last term in Eq. (2.5) was large and showed large variations for a series of functions $u_{\varepsilon lt}$ ranging from a two parameter to an eleven parameter function with u_t that given by Seaton.[4] The failure of this method in the particularly favorable e^-H case indicates that Eq. (2.5) is not a useful form. However, from Eq. (2.5) one can obtain an expression which does not depend on the unknown function $u_{\varepsilon l}$ by writing

$$\varepsilon_1\left(\int u_t u_{\varepsilon l}\,dr\right)^2 = \frac{1}{\varepsilon_1}\left(\int u_t \mathcal{L} u_{\varepsilon l}\,dr\right)^2$$

$$= \frac{1}{\varepsilon_1}\left(\int u_{\varepsilon l} \mathcal{L} u_t\,dr\right)^2 \leq \frac{1}{\varepsilon_1}\int (\mathcal{L} u_t)^2\,dr\ ,$$

where use has been made of the Schwarz inequality. We then obtain

$$A \leq A_t - \int u_t \mathcal{L} u_t\,dr + \frac{1}{\varepsilon_1}\int (\mathcal{L} u_t)^2\,dr\ . \tag{2.6}$$

The experimental value of the binding energy, if available, gives ε_1. Alternatively, ε_1 may be replaced by

$$\varepsilon_{1t} = \int u_{\varepsilon lt} \mathcal{L} u_{\varepsilon lt}\,dr \leq \varepsilon_1,$$

where $u_{\varepsilon lt}$ is a normalized trial bound state function, while still preserving the inequality, Eq. (2.6). For the case of scattering by a center of force, where quite accurate trial scattering functions may be constructed without great difficulty, Eq. (2.6) may be expected to give useful upper

bounds on A. However, the use of the Schwarz inequality in passing from Eq.(2.5) to Eq. (2.6) leads to a very great overestimate of the error term for any but an excellent u_t. Thus, the trial function given by Seaton for the singlet e^-H problem[4], which is expected to be reasonably accurate, leads nevertheless, when used in the appropriate generalization of Eq. (2.6) to scattering by a compound system, to an upper bound on the scattering length which is so large as to be quite useless. It does not seem that there exist other many body scattering problems for which a similar treatment would yield more favorable results.

It was therefore necessary to consider a somewhat different approach to the problem, one leading to a bound on A which does not require a knowledge of the exact composite bound state function and which does not utilize the often very crude Schwarz inequality. We now show how such a result can be obtained based on the following two theorems[5] which, for the purposes of later generalization, are quoted in a more general form than is needed in this section.

Theorem 1: We consider a system with exactly N bound states. If a KxK matrix of the Hamiltonian operator H is formed (K may be larger than, equal to or smaller than N) using a set of K orthonormal functions, and is diagonalized, with the diagonal elements arranged in increasing order, i.e.,

$$E_1^{(K)} \leq E_2^{(K)} \leq \cdots E_i^{(K)} \leq \cdots \leq E_K^{(K)},$$

then $E_i^{(K)} \geq E_i$, if $i \leq N$. Here E_i is the energy of the $i^{\underline{th}}$ bound state. For $i > N$, we have $E_i^{(K)} \geq 0$.

Theorem 2: If the Hamiltonian matrix is constructed in the same way as discussed in Theorem 1, but of rank K + 1 with the first K functions unaltered, then the eigenvalues, $E_i^{(K+1)}$, satisfy the relations

$$E_i \leq E_i^{(K+1)} \leq E_i^{(K)} .$$

We now apply these theorems to the case where only one bound state exists. We introduce the orthonormal functions v_1 and v_2 and form the 2x2 Hamiltonian matrix

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

where

$$H_{ij} \equiv (v_i, Hv_j), \qquad i,j = 1,2.$$

It is assumed that v_i is a sufficiently accurate ground state trial function[6] so that

$$H_{11} \equiv E_1^{(1)} < 0.$$

(If this last inequality is not satisfied, the method described below will not be applicable. This, however, does not represent a serious limitation since a trial function with the required accuracy can almost always be found.) It then follows that the eigenvalues of the above matrix, $E_1^{(2)}$ and $E_2^{(2)}$, satisfy the relations

$$E_2^{(2)} \geq 0,$$

from Theorem 1, and

$$E_1^{(2)} \leq E_1^{(1)} < 0,$$

from Theorem 2, so that

$$E_1^{(2)} E_2^{(2)} \leq 0.$$

Since the product of the eigenvalues of a matrix is equal to the determinant of the matrix we obtain the inequality

$$H_{11}H_{22} - H_{12}^2 \leq 0. \tag{2.7}$$

We note that since v_2 appears exactly twice in each of the two terms of this

inequality, neither the magnitude nor the sign of the normalization of v_2 is relevant, though of course v_2 must be normalizable. (Clearly the same is true of v_1 but it will be convenient in the following to think of v_1 as normalized to unity.) We now observe that the inequality, Eq. (2.7), is valid if v_2 is replaced by a normalizable function v_2' which is not orthogonal to v_1. This is verified by writing

$$v_2 = v_2' - (v_2', v_1)v_1 ,$$

[so that $(v_2, v_1) = 0$ is satisfied] and substituting this expression for v_2 in the integrals which appear in Eq. (2.7). Since the normalization of v_2' as well as the value of (v_2', v_1) are both arbitrary, as is clear from the above discussion, we are now in the position to choose

$$v_2' = w(\lambda) \equiv we^{-\lambda r} ,$$

with $\lambda > 0$. We then have the inequality which is the new form of Eq. (2.7),

$$\int w(\lambda) \mathcal{L} w(\lambda) dr \leq \frac{1}{\varepsilon_{1t}} \left(\int u_{\varepsilon 1t} \mathcal{L} w(\lambda) dr \right)^2 , \qquad (2.8)$$

with $\varepsilon_{1t} = -(2m/\hbar^2)E_1^{(1)}$ and $u_{\varepsilon 1t} = v_1$. Since both sides of the inequality, Eq. (2.8), are continuous at $\lambda = 0$ (see I) we have

$$\int w \mathcal{L} w dr \leq \frac{1}{\varepsilon_{1t}} \left(\int u_{\varepsilon 1t} \mathcal{L} w dr \right)^2 .$$

Therefore, since $\mathcal{L} w = \mathcal{L} u_t$, the expression which provides an upper bound on the scattering length becomes

$$A \leq A_t - \int u_t \mathcal{L} u_t dr + \frac{1}{\varepsilon_{1t}} \left(\int u_{\varepsilon 1t} \mathcal{L} u_t dr \right)^2 . \qquad (2.9)$$

We have then succeeded in our purpose in that we have obtained a bound which does not require a knowledge of the exact bound state function nor of its energy, and which has at the same time avoided the use of the rigorous but often very crude Schwarz inequality. (In the case where the scatterer is a compound system, the ground state wave function of the scatterer must still

be known exactly in order to obtain a rigorous bound.[7]) Note that the earlier results, Eqs. (2.5) and (2.6), may be considered as special cases of Eq. (2.9); the choice $u_{\varepsilon lt} = u_{\varepsilon l}$ in Eq. (2.9) yields Eq. (2.5), and the use of the Schwarz inequality in the last integral of Eq. (2.9) leads back to Eq. (2.6). It is of course clear that for a given form of the trial functions u_t and $u_{\varepsilon lt}$ the optimum choice of the variational parameters is such as to minimize the right hand side of Eq. (2.9), subject to the requirement that $\int u_{\varepsilon lt} \mathcal{L} u_{\varepsilon lt} dr > 0$.

For the case of arbitrary values of the orbital angular momentum, L, the inequality which corresponds to that given in Eq. (2.9) has the same form as the result for L = 0. We merely replace A (with a similar replacement of A_t) by A_L, defined in terms of the phase shift η_L as[1]

$$A_L = - [1x3x...x(2L+1)]^2 (\tan \eta_L / k^{2L+1})_{k=0} .$$

Further, the trial function, $u_{Lt}(r)$, satisfies the boundary conditions

$$u_{Lt}(0) = 0 ,$$
$$u_{Lt}(r) \to A_{Lt} r^{-L}/(2L+1) - r^{L+1}, \qquad \text{for} \quad r \to \infty,$$

and $\mathcal{L}$ now contains the additional term $L(L+1)/r^2$. Of course for a particular value of L the bound state considered is one with orbital angular momentum L. These results for arbitrary values of L can be extended in a straightforward manner to the case of scattering of one compound system by another, where each system may carry a net charge. The regular and irregular solutions of the "free" wave equation in the limit of vanishing energy have previously been given for this general case[8]. The asymptotic form of the wave function is taken as the "appropriate" linear combination of these solutions. The analysis then proceeds in a manner similar to that already described in I and II and we shall omit further details here.[9]

III. CONNECTION WITH FORMS OF THE VARIATIONAL PRINCIPLE

The inequality, Eq. (2.9), has the particular consequence that there exist well defined circumstances, which will now be described, under which an upper bound on the scattering length may be obtained from an ordinary variational calculation. (As in Section II the discussion in this section will be confined to the case where only one bound state exists.) We consider first the Kohn-Hulthén principle, which has the zero energy form

$$A \approx A_t - \int u_t \mathcal{L} u_t dr, \tag{3.1}$$

where u_t satisfies the boundary conditions given in Eqs. (2.2). Now suppose u_t may be written,

$$u_t = u_t' + b u_{\varepsilon lt}, \tag{3.2}$$

where $u_{\varepsilon lt}$ is a trial bound state function which is sufficiently accurate to give binding, i.e.,

$$\varepsilon_{lt} = \int u_{\varepsilon lt} \mathcal{L} u_{\varepsilon lt} \, dr > 0.$$

Since $u_{\varepsilon lt}$ vanishes at the origin and at infinity, u_t' satisfies the same boundary condition as u_t and can therefore itself serve as a proper trial scattering function. Substituting this form for u_t into the variational expression, Eq. (3.1), and determining b variationally, with u_t' and $u_{\varepsilon lt}$ momentarily considered as fixed, we find

$$b = -\frac{1}{\varepsilon_{lt}} \int u_{\varepsilon lt} \mathcal{L} u_t' \, dr,$$

and

$$A \approx A_t - \int u_t' \mathcal{L} u_t' \, dr + \frac{1}{\varepsilon_{lt}} \left(\int u_{\varepsilon lt} \mathcal{L} u_t' \, dr \right)^2. \tag{3.3}$$

It follows from Eq. (2.9) that the variational estimate of A given by Eq. (3.3) is actually an upper bound. Conversely, the approximation to the zero energy scattering function, obtained in the course of a calculation of an upper bound

on A based on Eq. (2.9), should be taken to be

$$u_t - \left(\frac{1}{\epsilon_{lt}} \int u_{\epsilon lt} \mathcal{L} u_t \, dr \right) u_{\epsilon lt}$$

rather than u_t since it is the former function which can be interpreted as a variationally determined trial function. We note that the prescription given by Kohn to evaluate the variational parameters should be used rather than that of Hulthén since, while both methods will provide an upper bound, for a given form of the trial function the Kohn method will yield a lower (and therefore better) estimate of the scattering length. (See I.)

It is of interest to see if there are any variational calculations of scattering lengths reported in the literature which were performed with trial functions which may be written in the form given by Eq. (3.2). Such calculations may be reinterpreted in the light of the present discussion. As an example we note that Borowitz and Greenberg[10] have recently performed a variational calculation for electron-hydrogen scattering, using as a zero energy trial function one which was explicitly constructed to be of the form of a trial scattering function plus a multiple of a trial H^- bound state function. Since the normalization used by these authors corresponds to what we have called the inappropriate normalization [see Eq. (2.4)] neither the results for the singlet case, where one bound state of H^- exists, nor for the triplet case, where no bound states exist, is necessarily a bound. However, as described in I, for those calculations which have been performed using the inappropriate normalization the results may be converted, with a trivial amount of labor, so that they correspond to the Kohn-Hulthén form and therefore do give a bound under the circumstances considered. The method of conversion may be briefly restated as follows. If A_t and $I \equiv \int u_t \mathcal{L} u_t \, dr$ have been evaluated,

with u_t normalized as in Eq. (2.4), then the bound on A is given by

$$A \leq A_t - A_t^2 I.$$

If A_t is positive and $|A_t I|$ is small compared to unity then this conversion may be expected to give, in addition to a bound, an improved approximation to the scattering length.

Returning to the work of Borowitz and Greenberg, we note that two separate calculations of the singlet scattering length[11] were performed, using two trial H^- functions obtained by Chandrasekhar[12]. One of these was a two parameter function containing no dependence on the interelectronic distance, r_{12}, so that no polarization was allowed for. The other function, which included a linear r_{12} dependence, contained three parameters. In each case the parameters used where those given by Chandrasekhar. The two and three parameter functions give values of ε_{1t} equal to 0.0266 a_o^{-2} and 0.0518 a_o^{-2} respectively[12] (a_o is the Bohr radius). The rigorous uppper bounds obtained by the conversion process described above yielded,in both cases, slightly improved approximations to the scattering length (see Table I).

IV. AN ALTERNATE METHOD

In this section we consider an alternate method for obtaining upper bounds on the scattering length for the case of the scattering of a particle by a center of force where one bound state exists. The method is based on the formalism given by Kato[13] for finding upper and lower bounds on the scattering phase shift. (Since the Kato method, as opposed to the Kato identity, is unrelated to the other methods discussed in this paper, this section may be read independently of the others.)

The Kato identity for arbitrary scattering energy, $(\hbar k)^2/2m$, of which Eq. (2.1) is the zero energy form with the normalization $0 < \theta < \pi$ (i.e., $\theta \neq 0$), is

$$k \cot(\eta - \theta) = k \cot(\eta_t - \theta) - \int u_{\theta t} \mathcal{L} u_{\theta t} dr + \int w_\theta \mathcal{L} w_\theta dr, \quad (4.1)$$

where now

$$\mathcal{L} = \frac{d^2}{dr^2} - (2m/\hbar^2) V(r) + k^2 .$$

The exact solution, u_θ, satisfies the differential equation $\mathcal{L} u_\theta = 0$, and the boundary conditions

$$u_\theta(0) = 0 ,$$
$$u_\theta(r) \to \sin(kr + \eta)/\sin(\eta - \theta) , \quad \text{for } r \to \infty , \quad (4.2)$$

where η is the exact phase shift and where θ satisfies $0 \leq \theta < \pi$. The trial function, $u_{\theta t}$, satisfies boundary conditions of the form given in Eqs. (4.2), but with η replaced by a trial phase shift, η_t, which is arbitrary; w_θ is defined as $u_{\theta t} - u_\theta$. The Kato inequalities are

$$-\alpha_\theta^{-1} \int (\mathcal{L} u_{\theta t})^2 \rho^{-1} dr \leq \int w_\theta \mathcal{L} w_\theta dr \leq \beta_\theta^{-1} \int (\mathcal{L} u_{\theta t})^2 \rho^{-1} dr. \quad (4.3)$$

Here $\rho(r)$ is a non-negative function which must fall off faster than $1/r$ but which is otherwise arbitrary and is chosen for convenience. The numbers α_θ and β_θ are defined by the associated eigenvalue problem, in which the equation

$$(\mathcal{L} + \mu\rho)\phi_\theta(r) = 0$$

is considered. The asymptotic form of $\phi_\theta(r)$ is characterized by a phase shift, $\delta(\mu)$. The infinite, discreet set of eignevalues, $\{\mu_{n\theta}\}$, is defined such that for any integer, n,

$$\delta(\mu_{n\theta}) = \theta + n\pi .$$

The smallest positive eigenvalue is α_θ and the largest negative eigenvalue is $-\beta_\theta$.

For zero energy scattering the phase shift in the associated eignevalue problem, $\delta(\mu)$, is given, according to a theorem due to Levinson,[14] by

$\delta(\mu) = m\pi$, if there is no state of exactly zero energy, where m is the number of bound states for the operator $\mathcal{L} + \mu\rho$. [If there are m bound states and there is one at zero energy in addition, the phase shift is $(m+\frac{1}{2})\pi$.] We are considering the case for which there is one and only one bound state for the actual physical system, i.e., for $\mu = 0$. We choose $\theta = \gamma$, where $0 < \gamma < \pi$. (The point is that we wish to exclude $\theta = 0$; note that the eigenvalues μ_{n0} do not form a discreet set at zero energy.) It is then clear that $-\beta_\gamma$ is determined by the condition that the operator $\mathcal{L} - \beta_\gamma\rho$ has associated with it a single, zero energy bound state. Actually, according to Eq. (4.3), only a lower bound on β_θ is required in order to obtain an upper bound on $\int w_\theta \mathcal{L} w_\theta dr$. Now a lower bound on β_γ is easily determined, according to the Rayleigh-Ritz principle, by

$$\int \psi_t [\mathcal{L} - \beta_\gamma \rho] \psi_t dr \leq 0,$$

where ψ_t is an arbitrary normalized trial bound state function. We have

$$\beta_\gamma \geq \int \psi_t \mathcal{L} \psi_t dr / \int \psi_t^2 \rho dr \equiv \beta_\gamma'. \tag{4.4}$$

This result is useful only if $\beta_\gamma' > 0$, that is, ψ_t must be sufficiently accurate such that $(\psi_t, \mathcal{L}\psi_t) > 0$.

If we take the zero energy form of Eq. (4.1), with $\theta = \gamma$, and make use of Eqs. (4.3) and (4.4), we obtain

$$A \leq A_t - \int u_t \mathcal{L} u_t dr + (\beta_\gamma')^{-1} \int (\mathcal{L} u_t)^2 \rho^{-1} dr, \tag{4.5}$$

where

$$A \equiv -(\tan\eta/k)_{k=0},$$

$$A_t \equiv -(\tan\eta_t/k)_{k=0},$$

$$u_t \equiv (u_{\gamma t}/k)_{k=0}$$

and where β_γ' is defined in Eq. (4.4).

A number of methods have been given previously[13,15] for determining lower bounds on α_Θ and β_Θ, for arbitrary scattering energy. The method just described, while limited to zero energy scattering, has the virtue that the prescription for finding a bound on β_Θ is quite general. The potential need satisfy no special requirements other than that it lead to one bound state[16], and that a phase shift be defined. This generality becomes quite significant in the case of scattering by a compound system, where methods based on special properties of the potential (such as being everywhere negative, for example) will usually be inapplicable. However, serious problems arise in the extension of Levinson's theorem to the case of scattering by a compound system, and as discussed briefly in I, the inclusion of the Pauli principle raises additional difficulties. Therefore, until these questions are clarified the method presented in this section should be used only for one body scattering problems.

It is noted that α_γ, which is required to obtain a lower bound on A, is determined as that value of μ for which the second bound state appears. Now for a static potential, U(r), the necessary condition for the existence of n_L bound states, of orbital angular momentum L, is[17]

$$(2m/\hbar^2) \int r|U(r)|dr > (2L+1)n_L \ . \qquad (4.6)$$

In the case being considered, where the actual potential, V(r), supports one bound state with L = 0, we have from Eq. (4.6) that α_γ', determined by

$$\int r|-(2m/\hbar^2)V(r) + \alpha_\gamma' \rho(r)|dr = 2 \ ,$$

is a lower bound on α_γ. This result will be useful only if $\alpha_\gamma' > 0$. In particular, a necessary condition for the applicability of the method is

$$-(2m/\hbar^2) \int r\, V(r)dr < 2 \ .$$

An obvious disadvantage of this approach is that (contrary to the method for determining β_γ') it provides no way of successively improving the bound on α_γ. Further, even if Levinson's theorem can be shown to hold in the case of scattering by a compound system, no generalization of Eq. (4.6) has been obtained; there would still remain the problem of determining conditions for the non-existence of many body bound states.

V. THE CASE OF MORE THAN ONE BOUND STATE

The generalization of the above results to the case for which there is more than one bound state of zero angular momentum of the particle and the center of force is fairly straightforward. We assume that it is known that there exist exactly N such bound states. The exact eigenfunctions and the exact energies of these states will be denoted by $u_{\varepsilon 1}$ through $u_{\varepsilon N}$ and by E_1 through E_N, respectively, where

$$E_1 < E_2 < \cdots E_N < 0 ,$$

and $\varepsilon_i \equiv (2m/\hbar^2)E_i$, $1 \leq i \leq N$. We do not assume that the eigenfunctions or the eigenvalues are actually known.

The generalization of Eq. (2.6) is particularly simple. Since the function

$$w' \equiv w - \sum_{i=1}^{N} (w, u_{\varepsilon i})u_{\varepsilon i}$$

is orthogonal to each of the bound states, it follows that

$$\int w' \mathcal{L} w' dr \leq 0,$$

where it is assumed that the "appropriate" normalization, namely that given by Eq. (2.2), has been used. Substituting for w', we find

$$\int w \mathcal{L} w \, dr \leq \sum_{i=1}^{N} \frac{1}{\varepsilon_i} \left(\int u_{\varepsilon i} \mathcal{L} u_t dr\right)^2 .$$

The elimination of the unknown $u_{\varepsilon i}$ by the Schwarz inequality leads to

$$\int w \mathcal{L} w \, dr \leq \left(\sum_{i=1}^{N} \frac{1}{\varepsilon_i} \right) \int (\mathcal{L} u_t)^2 dr \, .$$

However, an improved bound may be obtained by writing

$$\sum_{i=1}^{N} \frac{1}{\varepsilon_i} \left(\int u_{\varepsilon i} \mathcal{L} u_t dr \right)^2 \leq \frac{1}{\varepsilon_N} \sum_{i=1}^{N} \left(\int u_{\varepsilon i} \mathcal{L} u_t dr \right)^2 \leq \frac{1}{\varepsilon_N} \sum_{i=1}^{\infty} \left(\int u_{\varepsilon i} \mathcal{L} u_t dr \right)^2 ,$$

where the summation in the last term (which actually includes an integration over continuum functions) is over the complete set of energy eigenfunctions. Making use of the closure property of this set we have

$$\int w \mathcal{L} w dr \leq \frac{1}{\varepsilon_N} \int (\mathcal{L} u_t)^2 dr \, , \tag{5.1}$$

so that

$$A \leq A_t - \int u_t \mathcal{L} u_\varepsilon dr + \frac{1}{\varepsilon_N} \int (\mathcal{L} u_t)^2 dr \, . \tag{5.1}'$$

If ε_N is unknown, a lower bound may be employed, obtained, for example, by the method described in Theorem 1.

An alternate proof[18] of Eq. (5.1) may be based on the inequality[19]

$$\int \psi_t (H-c)^2 \psi_t \, dr \geq (E_c - c)^2 \int \psi_t^2 \, dr \, , \tag{5.2}$$

which is verified by substituting the energy eigenfunction expansion for the normalizable trial function, ψ_t; c is an arbitrary non-positive energy value and E_c is the energy eigenvalue closest to c. The inequality, Eq.(5.1), follows from the choice $c = E_N/2$.

To obtain the generalization of the more useful result, Eq. (2.9), we introduce N orthonormal functions and construct and diagonalize the N x N

matrix of the operator H, as discussed in Theorem 1. The N eigenvalues of the matrix will again be denoted by $E_i^{(N)}$, while the N orthonormal eigenvectors of the matrix determine N orthonormal eigenfunctions; the latter will be denoted by $v_i(r)$. It is assumed that the trial functions $v_i(r)$ are sufficiently accurate so that

$$E_i^{(N)} < 0 \quad , \qquad 1 \leq i \leq N. \tag{5.3}$$

We now introduce an additional trial function, $v_{N+1}(r)$, which is normalized and which is orthogonal to each of the $v_i(r)$, $1 \leq i \leq N$. With this set of N + 1 orthonormal functions, we construct an (N+1) x (N+1) matrix from the operator H. Since the determinant of a matrix is equal to the product of its eigenvalues, we have

$$\begin{vmatrix} E_1^{(N)} & & & H_{1,N+1} \\ & E_2^{(N)} & & H_{2,N+1} \\ & & \ddots & \vdots \\ H_{N+1,1} & H_{N+1,2} & \cdots & H_{N+1,N+1} \end{vmatrix} = E_1^{(N+1)} \times E_2^{(N+1)} \times \ldots E_{N+1}^{(N+1)} . \tag{5.4}$$

In the above determinant all the elements not on the diagonal nor in the last row nor last column are equal to zero, and we have

$$H_{N+1,i} = H_{i,N+1} = \int v_i \, H \, v_{N+1} \, dr \quad , \qquad 1 \leq i \leq N+1;$$

the $E_i^{(N+1)}$, $1 \leq i \leq N+1$, are the N+1 ordered eigenvalues of the matrix. Since we have introduced an additional trial function, it follows from Theorem 2 that $E_i^{(N+1)} \leq E_i^{(N)}$, $1 \leq i \leq N$, and therefore, from Eq. (5.3), that

$E_i^{(N+1)} \leq 0$ for $1 \leq i \leq N$. On the other hand, since there are only N bound states, it follows from Theorem 1 that $E_{N+1}^{(N+1)} \geq 0$.

Now the expansion of the determinant in Eq. (5.4) leads to

$$H_{N+1,N+1} = \sum_{i=1}^{N} \frac{1}{E_i^{(N)}} (H_{i,N+1})^2 + \frac{E_1^{(N+1)}}{E_1^{(N)}} x \cdots \frac{E_N^{(N+1)}}{E_N^{(N)}} x E_{N+1}^{(N+1)}.$$

Since from the previous discussion $E_i^{(N+1)}/E_i^{(N)} > 0$ for $1 \leq i \leq N$ and $E_{N+1}^{(N+1)} \geq 0$, we have the inequality

$$H_{N+1,N+1} \geq \sum_{i=1}^{N} \frac{1}{E_i^{(N)}} (H_{i,N+1})^2. \tag{5.5}$$

It is clear from this last inequality that while v_{N+1} must be normalizable, its specific normalization is irrelevant. We choose for v_{N+1} a function which, as required, is orthogonal to the v_i, $1 \leq i \leq N$, i.e.,

$$v_{N+1} = w - \sum_{i=1}^{N} (w, v_i) v_i . \tag{5.6}$$

The difference function w must be thought of as normalizable, but need not be orthogonal to the v_i. Eq. (5.5) then becomes

$$\int w H w \, dr \geq \sum_{i=1}^{N} \frac{1}{E_i^{(N)}} \left(\int v_i H u_t \right)^2 dr, \tag{5.7}$$

using $H w = H u_t$, or, equivalently,

$$\int w \mathcal{L} w \, dr \leq \sum_{i=1}^{N} \frac{1}{\varepsilon_i^{(N)}} \left(\int v_i \mathcal{L} u_t dr \right)^2. \tag{5.7}'$$

We now obtain from this the generalization that we want, namely,

$$A \leq A_t - \int u_t \mathcal{L} u_t dr + \sum_{i=1}^{N} \frac{1}{\varepsilon_i^{(N)}} \left(\int v_i \mathcal{L} u_t dr \right)^2 . \tag{5.8}$$

We might note that Eq. (5.7) is of precisely the same form as Eq. (5.5), with v_{N+1} replaced by w. This invarience can perhaps be better understood

by recognizing that the earlier determinantal equation, Eq. (5.4), is invariant under the same transformation. Thus, the transformation from $v_1,\ldots,v_N,v_{N+1}$ to $v_1,\ldots,v_N,w$, where v_{N+1} is defined by Eq. (5.6), is given by the transformation matrix $\underset{\sim}{B}$, where

$$\underset{\sim}{B} = \begin{pmatrix} 1 & & \\ & 1 & \\ (w,v_1) & (w,v_2) & \cdots 1 \end{pmatrix}.$$

The invariance of the determinantal equation, Eq. (5.4), under the substitution $v_{N+1} \rightarrow w$ is then guaranteed by the fact that $\underset{\sim}{B}$ is unimodular.

Finally, we note that the result of Section III is easily extended to the case of many bound states. That is, the right hand side of Eq. (5.8) may be identified with the Kohn-Hulthén expression for the scattering length, in which the trial function

$$u_t + \sum_{i=1}^{N} b_i v_i$$

is used, provided each of the b_i is determined variationally.

VI. DISCUSSION

The two principle results that have been derived, which enable one to calculate upper bounds on the scattering length for those problems in which a finite number of composite bound states exist, are expressed by the inequalities, Eqs. (5.1)' and (5.8). The inequality of Eq. (5.8) will lead to more accurate estimates of the scattering length than may be obtained from Eq. (5.1)'. The latter result does have one advantage in that one has removed the necessity of constructing a set of trial bound state functions and performing the various integrals involving these functions. However, it may be quite difficult, in

the more complicated problems, to construct a trial scattering function sufficiently accurate to obtain useful results from Eq. (5.1)'; the performance of the required integrals may also present formidable difficulties. Eq. (5.8) has the interesting consequence that certain ordinary variational calculations provide bounds.

As was mentioned in Section I, the results are derived in terms of the simple case of the zero orbital angular momentum scattering of a spinless, neutral particle by a center of force, but may be directly generalized to a far wider class of problems. The essential restriction which must be maintained is that only one exit channel (elastic scattering, including Pauli exchange) should be open. As an illustration we cite the extension of Eq. (5.8) for the problem of the scattering of a particle by a compound system. The appropriate inequality becomes

$$A \leq A_t - \int \Psi_t^* \Lambda \Psi_t \, d\tau + \sum_{i=1}^{N} \frac{1}{\epsilon_i} \left(\int \Phi_i^* \Lambda \Psi_t \, d\tau \right)^2. \qquad (6.1)$$

We have denoted the trial scattering function and the trial function for the $i^{\underline{th}}$ composite bound state by Ψ_t and Φ_i, respectively, instead of u_t and v_i merely to indicate that they represent the functions with no factors of $1/r$ separated out. The operator Λ is defined as $\Lambda = -(2\mu/\hbar^2)(H-E_g)$, where H is the total Hamiltonian, where E_g is the ground state binding energy of the scattering system, and where μ is the reduced mass for the scattered particle and the compound scatterer. If, asymptotically, there exists a net repulsive Coulomb interaction between the scattered particle and the scattering system then the inequality which is applicable is identical in form with that given in Eq. (6.1) but A is now defined in terms of the "additional" phase shift, η, as[20]

$$A \equiv -(\tan \eta / kC^2)_{k=0}$$

where C^2 is the Coulomb penetration factor. (The asymptotic form of the trial function, Ψ_t, is altered in this case but we shall omit further details here.)

There is a lack of completeness in the results obtained here in the sense that no method has been given, valid for many body scattering problems, which provides a lower bound on the scattering length. Such a method is clearly very much to be desired and work is now in progress on this aspect of the problem. On the other hand, while a single bound on the scattering length allows one, in a particular calculation, to make no rigorous error estimate whatsoever, and may provide neither bound on the zero energy cross section,[21] the knowledge that one has a minimum principle allows for successive improvements not only in the calculated scattering length but the trial wave function as well. Since an accurate estimate of the effective range, r_o, (but not the shape dependent parameter, P) may be obtained from an accurate zero energy trial function it can be said that the benefits obtained from doing the zero energy calculation based on a minimum principle may be utilized in the case of slightly higher energies as well. Numerical calculations for the problem of electron scattering by atomic hydrogen (for P and D, as well as S-wave scattering) are now being performed. It is hoped that with the aid of the present techniques the discrepencies regarding the total low energy e^-H scattering cross section, which have recently been reported, may be resolved.

Table I. Results of variational calculations of the singlet e^-H scattering length, in units of the Bohr radius. In the first column the values obtained by Borowitz and Greenberg, who used what we have called the 'inappropriate' normalization [see Eq. (2.4)], are given. The values which appear in the second column were obtained by the present authors by converting the Borowitz-Greenberg data to the Kohn-Hulthén form ['appropriate' normalization; see Eqs. (2.2)], thereby obtaining a rigorous upper bound. The fact that a slight improvement is gained in this conversion is in agreement with the discussion in the text. It was possible to obtain a bound because the u_t used by the above authors included a bound state component multiplied by a variational parameter.

	NORMALIZATION	
	'INAPPROPRIATE'	'APPROPRIATE'
NO POLARIZATION APPROXIMATION	8.16	8.14
POLARIZATION CONSIDERED	7.75	7.63

REFERENCES

1 L. Spruch and L. Rosenberg, submitted for publication in the Physical Review. This paper will be referred to in the following as I.

2 L. Spruch and L. Rosenberg, submitted for publication in the Physical Review. This paper will be referred to in the following as II.

3 Actually, the neglect of the radiative capture process is not valid at zero energy since it obeys a 1/v law. However, the coefficient of 1/v is sufficiently small so that the capture process is negligible compared to the probability for elastic scattering for all but the lowest energies. The calculated scattering length may then be interpreted as an extrapolation from some small, non-zero energy value.

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6 It would be more consistent to denote this trial function as $u_{\varepsilon 1t}$ (as is done later on in this section). For the present, however, we use the simpler notation v_1. In Section V, where the case of many bound states is considered, we label the trial bound state functions by v_i rather than $u_{\varepsilon it}$, again for simplicity of notation.

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Research Reports and Publications

The following is a list of all research reports in the CX series:

CX-1	S. Borowitz	The Schwinger Variational Method for Three-Body Collisions Published - Borowitz and Friedman Phys. Rev., 89, 441 (1953). Math. Rev., 14, 756 (1953).	April'52
CX-2	H. Moses	A Self-Consistent Calculation of the Dissociation of Oxygen in the Upper Atmosphere Published - Phys. Rev., 87, 628 (1952).	April'52
CX-3	K. Wildermuth	A Rigorous Solution of a Many-Body Problem Published - Acta Physica Austriaca, 7, 299 (1953).	Aug.'52
CX-4	B. Friedman and E. Gerjuoy	Scattering Problems in Nonrelativistic Quantum Mechanics; Part I - One Particle in One Dimension	Dec.'52
CX-5	H. Moses	Exchange Scattering in a Three-Body Problem Published - Phys. Rev., 91, 185 (1953). Math. Rev., 16, 1186 (1955).	Jan.'53
CX-6	H. Moses	Formulation of the Kohn-Hulthén Variational Principle in Terms of the Scattering Operator Formalism Published - Phys. Rev., 92, 817 (1953). Math. Rev., 15, 587 (1954).	April'53
CX-7	H. Boyet and S. Borowitz	A Variational Calculation of the Elastic Scattering of Electrons by Hydrogen Atoms Published - Phys. Rev., 93, 1225 (1954).	April'53
CX-8	H. Moses	A Self-Consistent Calculation of the Dissociation of Oxygen in the Upper Atmosphere; Part II- Three Body Recombinations Published - Phys. Rev., 91, 1408 (1953).	April'53
CX-9	E. Bauer and Ta-You Wu	The Origin of the E-Layer of the Ionosphere Published - Phys. Rev., 92, 1101 (1953).	July '53

CX-10	J.B. Keller	Derivation of the Bohr-Sommerfeld Quantum Conditions from an Asymptotic Solution of the Schrödinger Equation Published - Annals of Physics, 4, 180 (1958).	July '53
CX-11	E. Bauer	Self-Consistent Field Equations for H_2 and H_3	Aug. '53
CX-12	H. Moses	The Scattering Operator in Quantum Mechanics; Part I - The Properties of the Scattering Operator from the Time-Dependent Schrödinger Equation (see CX-13) Math. Rev., 16, 1186 (1955).	Oct. '53
CX-13	H. Moses	The Scattering Operator in Quantum Mechanics; Part II- The Scattering Operator Formalism and Other Formalisms Published - (CX-12 and CX-13, portion of the material) Phys. Rev., 96, 519 (1954). Published - (CX-12 and CX-13, summary) Il Nuovo Cimento, 1, 103 (1955). Math. Rev., 16, 1187 (1955).	Dec. '53
CX-14	E. Bauer and Ta-You Wu	The Cooling of a Gas by Radiation Published - Proc. Phys. Soc. of London, A 67, 741 (1954).	April '54
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CX-16	S. Borowitz	A Perturbation Calculation of the Elastic Scattering of Electrons by Hydrogen Atoms Published - Phys. Rev., 96, 1523 (1954).	June '54
CX-17	E. Bauer	A Method of Calculating Cross Sections for Molecular Collisions Published - J. Chem. Phys., 23, 1087 (1955).	Oct. '54
CX-18	H. Moses and I. Kay	The Determination of the Scattering Potential from the Spectral Measure Function Published - Il Nuovo Cimento, 2, 917 (1955). Math. Rev., 16, 929 (1955). Math. Rev., 17, 372 (1956).	Jan. '55

CX-19	H. Moses and I. Kay	The Determination of the Scattering Potential from the Spectral Measure Function; Part II- Point Eigenvalues and Proper Eigenfunctions Published - Il Nuovo Cimento, 3 66 (1956). Math. Rev., 17, 155 (1956). Math. Rev., 17, 740 (1956).	June '55
CX-20	H. Moses and I. Kay	The Determination of the Scattering Potential from the Spectral Measure Function; Part III - Calculation of the Scattering Potential from the Scattering Operator for the One-Dimensional Schrödinger Equation Published - Il Nuovo Cimento, 3, 276 (1956). Math. Rev., 17, 489 (1956).	Sept. '55
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List of Publications Not Based on Reports

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